

Non-local interactions in a BEC: Perturbative energy functional and the dispersion relation.

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We consider a Gross-Pitaevskii(GP) model of Bose-Einstein Condensate(BEC) with non-local s-wave scattering. In this model we use the Taylor expansion of the wavefunction in the interaction term of the GP equation. We show an interesting property of this expansion which allows us to truncate the Taylor series of the energy functional too, up to the same order as the truncation of the corresponding equation for dynamics which can be obtained by variation of the energy functional. Further we show analytically the existence of roton minimum in the spectrum of elementary excitations on top of the uniform density ground state in such a system under the condition that the range of interparticle interaction be greater than the average particle separation.

INTRODUCTION

Since the realisation of BEC in atomic gases[6], a lot of study has emerged on various aspects of BEC like quantized vortices, solitons, etc. The chief method of treatment of BEC in dilute atomic gases is using the mean field Gross-Pitaevskii(GP) equation where the interaction between bosons is that of contact type. Non-local interactions usually come into play in the theory when considering dipolar BEC. It is interesting to study the GP equation in the presence of extended interactions rather than point interactions, while still staying in the symmetric scattering regime. In this direction, there are a lot of studies which introduce a correction term of the form $\psi \nabla^2 |\psi|^2$ by hand to the local GP equation. Some studies have derived the correction terms from the interaction term in the GP equation[16, 17]. We had suggested that instead of introducing a term by hand, it would be informative to obtain a perturbative series from the GP equation and truncate the series to desired accuracy depending on the coefficients of the expansion and higher order derivatives of $|\psi|^2$ [4]. But the question of obtaining an energy functional for such an expansion remains, which at first sight doesn't seem straightforward to answer.

It is also interesting to study the spectrum of elementary excitations on top of the uniform density ground state in the presence of non-local interactions. The spectrum of elementary interactions using contact interactions between the constituent bosons exhibit the phonon spectrum at long wavelengths and free particle behaviour at small wavelengths in the dispersion relation, but the roton minimum doesn't show. Since the BEC is a superfluid as long as the Landau criterion is satisfied, it is but natural to ask whether a roton minimum like in the case of liquid He II is present in a BEC. The main difference between BEC in dilute gases and superfluid He II is the huge difference in the density and the range of interactions. This observation naturally raises a curious question as to what would happen if in a non-dipolar

BEC we consider not just contact interactions, but extended or non-local interactions in the low energy limit of the s-wave interactions.

Since the phenomenological two liquid model proposed by Landau [5], the quantitative features of superfluid He II have been attributed to the existence of the roton minimum. It has been shown that a BEC too exhibits the property of superfluidity when the Landau criterion is satisfied[8]. The excitation spectrum proposed by Landau for superfluid helium II has been put to the test experimentally and a roton minimum has been observed in He II by neutron scattering experiments [2]. Similarly, in a BEC Bragg Spectroscopy enables to observe the spectrum of elementary excitations experimentally in a BEC[12, 13]. It has been proposed that in the presence of long range interactions and by increasing their strength roton minimum may be observed in a BEC[10, 11]. It has also been recently observed experimentally that spin-orbit coupling in a BEC[14] and shaken optical lattices[15] can also lead to a roton minimum in the excitation spectrum.

In the first part of this article we take a non-local interaction potential between bosons and expand the interaction term in the GP equation using a Taylor series. We truncate the Taylor series to an arbitrary order. For this truncated series, we try to find out an energy functional whose variation will give us the truncated GP equation. We show an interesting mathematical result that the energy functional from which the truncated GP equation can be obtained can itself be obtained by truncating the Taylor series of the general GP energy functional upto the exact same order as that of the corresponding truncated GP equation.

In the second part, we consider the mean field GP equation with non-local, symmetric Gaussian interaction between bosons which interact via s-wave scattering. We consider the uniform density ground state $\psi(\mathbf{r}, \mathbf{t}) = \sqrt{n} e^{-i\mu t/\hbar}$ and study the spectrum of linear elementary excitations on top of this state. We show that due to the non-local interactions, the spectrum of elementary excitations shows a roton minimum and mim-

ics the phenomenological curve of elementary excitations postulated by Landau[1].

SERIES EXPANSION OF GP EQUATION

The general GP equation for a condensate is given as

$$i\hbar \frac{\partial \psi(\mathbf{r}, \mathbf{t})}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}, \mathbf{t}) + \psi(\mathbf{r}, \mathbf{t}) \int d\mathbf{r}' \psi^*(\mathbf{r}', \mathbf{t}) \mathbf{V}(\mathbf{r}' - \mathbf{r}) \psi(\mathbf{r}', \mathbf{t}). \quad (1)$$

The local form of the GP equation considers only contact type interactions between particles. This local form of the GP equation in the absence of external potential is

$$i\hbar \frac{\partial \psi(\mathbf{r}, \mathbf{t})}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}, \mathbf{t}) + g |\psi(\mathbf{r}, \mathbf{t})|^2 \psi(\mathbf{r}, \mathbf{t}). \quad (2)$$

These equations have been successful in explaining many properties of a BEC. We wish to look at the properties of Eq.(1) under non-local interactions. Since, we are considering s-wave interactions only, we have the benefit of using an effective, soft interparticle potential V_{eff} as long as it satisfies the criterion $\int V_{eff}(\mathbf{r}) d\mathbf{r} = g = \frac{4\pi\hbar^2 a}{m}$. We use this property and consider a potential which is gaussian having standard deviation equal to the s-wave scattering length. We will be considering here a condensate in the absence of an external potential.

A feature of symmetric non-local interactions that we studied is the series expansion of the wave-function and obtaining a modified GP equation and its corresponding energy functional. The series expansion of the GP equation has been previously presented by us with respect to density modulated states in a BEC[4]. In this expansion, there is an interesting property which shall be presented in the following. We shall discuss the case where the density is perturbed only along one axis and is uniform along the other two axes in cartesian coordinates for simplicity. The modified equation previously presented by us is of the form

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \partial_x^2 \psi(x, t) + g \psi(x, t) \left(|\psi(x, t)|^2 + \frac{a^2}{2} \partial_x^2 |\psi(x, t)|^2 + \frac{a^4}{8} \partial_x^4 |\psi(x, t)|^2 + \frac{a^6}{48} \partial_x^6 |\psi(x, t)|^2 + \dots \right) \quad (3)$$

This simple model can be derived from Eq.(1) by using gaussian interaction potential between particles and expanding $|\psi(\mathbf{r}')|^2$ in Taylor series around $\mathbf{r}' = \mathbf{r}$. Note that only even order derivatives would exist due to the symmetry of the gaussian potential used. In deriving the above equation we have taken a gaussian interaction potential. However note that any symmetric soft potential

$V_{eff}(\mathbf{r})$ with $\int V_{eff}(\mathbf{r}) d\mathbf{r} = g$ can be used.

Let us assume that the properties of a condensate can be explained upto the desired accuracy when we truncate the above series upto, say j th order in derivatives. Notice that as the interaction potential is symmetric, j is even. We observe that such an equation can be obtained by variation of the energy functional

$$F = \int d\vec{r} \left[\frac{\hbar^2}{2m} |\partial_x \psi|^2 + g \frac{|\psi(x, t)|^2}{2} \left(|\psi(x, t)|^2 + \frac{a^2}{2} \partial_x^2 |\psi(x, t)|^2 + \frac{a^4}{8} \partial_x^4 |\psi(x, t)|^2 + \dots + \frac{a^j}{j!!} \partial_x^j |\psi(x, t)|^2 \right) \right]. \quad (4)$$

Notice that the series in the above energy functional too is terminated upto the j th order in derivatives. An interesting thing which we noticed is the fact that there is an exact correspondence between the term $\frac{|\psi|^2}{2} \frac{\partial^l |\psi|^2}{\partial x^l}$ in the energy functional and the term $\psi \frac{\partial^l \psi}{\partial x^l}$ in the modified GP Eq.(3). Notice here that l was even. With an odd l , the correspondence between the l th order derivative in the energy functional and that in the modified GP equation is absent. An odd l can be obtained when the

interaction potential is not even, but with a non-definite parity such that the integral $\int (x - x')^l V_{eff}$ is non-zero, where $\int V_{eff} = g$. Notice that V_{eff} cannot be odd, since in that case it's integral would be zero and the criterion $\int V_{eff}(\mathbf{r}) d\mathbf{r} = g$ can't be satisfied. The proof of the correspondence between terms in the energy functional and that in the modified GP equation goes as follows.

Consider the term in the energy functional $G = \frac{|\psi|^2}{2} \partial_x^l |\psi|^2$. Let us look at the functional derivative of G with respect to ψ^* .

$$\begin{aligned}
\frac{\delta G}{\delta \psi^*} &= \left(\sum_{m=0}^l (-1)^m \partial_x^m \frac{\partial}{\partial (\partial_x^m \psi^*)} \right) \left[\frac{|\psi|^2}{2} \left(\sum_{n=0}^l \binom{l}{n} (\partial_x^{l-n} \psi) (\partial_x^n \psi^*) \right) \right] \\
&= \frac{\psi}{2} \partial_x^l (|\psi|^2) + \frac{1}{2} \left[\sum_{m=0}^l (-1)^m \binom{l}{m} \partial_x^m (|\psi|^2 (\partial_x^{l-m} \psi)) \right] \\
&= \frac{\psi}{2} \partial_x^l (|\psi|^2) + \frac{1}{2} \left[\sum_{m=0}^l (-1)^m \binom{l}{m} \sum_{p=0}^m \binom{m}{p} (\partial_x^p |\psi|^2) (\partial_x^{l-p} \psi) \right]
\end{aligned} \tag{5}$$

Let us fix p and considering the sum over m , look at the the second term on the right hand side in square brackets of the above equation, which becomes $\sum_{m=p}^l (-1)^m \binom{l}{m} \binom{m}{p} \partial_x^p |\psi|^2 \partial_x^{l-p} \psi$. Notice the lower sum

is from p and not zero. This is necessary, because to have a term with p -th derivative, the minimum necessary order of the differential operator is p . Also note that $p \leq m$. Let us introduce $q = m - p$. So we have,

$$\begin{aligned}
\sum_{m=p}^l (-1)^m \binom{l}{m} \binom{m}{p} (\partial_x^p |\psi|^2) (\partial_x^{l-p} \psi) &= \sum_{q=0}^{l-p} (-1)^{q+p} \binom{l}{q+p} \binom{q+p}{p} (\partial_x^p |\psi|^2) (\partial_x^{l-p} \psi) \\
&= \sum_{q=0}^{l-p} (-1)^{q+p} \binom{l}{p} \binom{l-p}{q} (\partial_x^p |\psi|^2) (\partial_x^{l-p} \psi) \\
&= (\partial_x^p |\psi|^2) (\partial_x^{l-p} \psi) (-1)^p \binom{l}{p} \sum_{q=0}^{l-p} (-1)^q \binom{l-p}{q},
\end{aligned}$$

where we have used the property $\binom{l}{q+p} \binom{q+p}{p} = \binom{l}{p} \binom{l-p}{q}$. It is easy to see that $\sum_{q=0}^{l-p} (-1)^q \binom{l-p}{q}$ is noth-

ing but the expansion of $(1-1)^{l-p}$, which is zero, except for the case when $p = l$, for which, from Eq.(5) we can see that, $m = l$. Using this information viz., $p = m = l$ Eq.(5) assumes the following form

$$\begin{aligned}
\frac{\delta G}{\delta \psi^*} &= \frac{\psi}{2} \partial_x^l (|\psi|^2) + \frac{1}{2} \left[(-1)^l \left(\psi (\partial_x^l |\psi|^2) \right) \right] \\
&= \left(\frac{\psi}{2} \partial_x^l |\psi|^2 \right) + (-1)^l \left(\frac{\psi}{2} \partial_x^l |\psi|^2 \right).
\end{aligned} \tag{6}$$

From this it is clear that $\frac{\delta}{\delta \psi^*} \left(\frac{|\psi|^2}{2} \partial_x^l |\psi|^2 \right) = \psi \partial_x^l (|\psi|^2)$ only when l is even and $\frac{\delta}{\delta \psi^*} \left(\frac{|\psi|^2}{2} \partial_x^l |\psi|^2 \right) = 0$ if l is odd. Note that the interaction potential need not be even. It would be sufficient if the interaction potential is integrable and doesn't allow odd order derivatives to be present for the correspondence between the perturbative energy functional and the modified GP equation to exist.

This result is very important in that it shows a preference towards interaction potentials which do not generate odd derivatives in the given Taylor expansion for the treatment of the GP equation perturbatively, where the energy functional is very straightforward to evaluate,

simply by expanding the GP energy functional and truncating it to the same order as the modified GP equation. Perturbation theory is not new to the field of Quantum Physics and has been successfully used to obtain approximate results for many a quantum phenomenon. Similarly, the expansion presented here can be used to obtain perturbative solutions to the GP equation in presence of extended interactions between constituent particles by truncating the series upto desired accuracy depending on the coefficients and conditions on behaviour of higher order derivatives of the wavefunction.

NON-LOCALITY AND THE ROTON MINIMUM

Now, let us consider the 3 dimensional BEC and take the interaction potential of the form $V_{eff}(\mathbf{r}' - \mathbf{r}) = \frac{g}{\sqrt{2\pi}a} e^{-\frac{|\mathbf{r}-\mathbf{r}'|^2}{2a^2}}$. Note that the uniform density state $\psi_0(\mathbf{r}, t) = \sqrt{n} e^{-i\mu t/\hbar}$ is still a solution of this non-local equation with $\mu = gn$ since the form of $\psi_0(\mathbf{r}, t)$ doesn't have a space dependent part to it. Hence we do not expect non-locality to affect the uniform density state. What would be interesting is to look at

$$\begin{pmatrix} \hbar\omega - \frac{\hbar^2 k^2}{2m} - gne^{-\frac{a^2 k^2}{2}} & -gne^{-\frac{a^2 k^2}{2}} \\ gne^{-\frac{a^2 k^2}{2}} & \hbar\omega + \frac{\hbar^2 k^2}{2m} + gne^{-\frac{a^2 k^2}{2}} \end{pmatrix} \begin{pmatrix} u_i \\ v_i \end{pmatrix} = 0. \quad (7)$$

Since we are looking for non-zero excitations, the determinant of the 2×2 matrix in the above equation should be zero. Setting the determinant equal to zero gives us the dispersion relation

$$\omega^2 = \frac{\hbar^2}{m^2} \left(\frac{k^4}{4} + 4\pi a n k^2 e^{-\frac{a^2 k^2}{2}} \right). \quad (8)$$

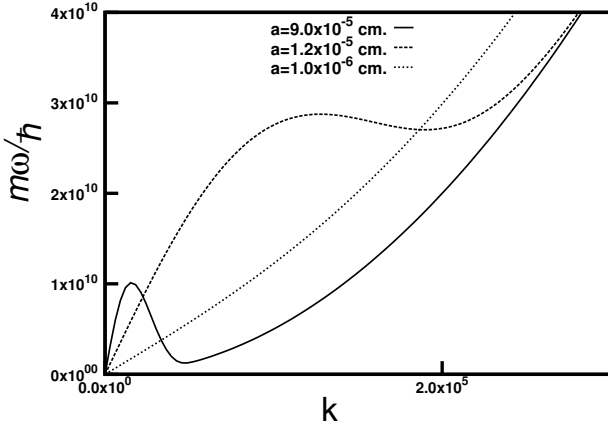


FIG. 1. Figure shows the dispersion relation at a fixed density of $n = 10^{15} \text{ cm}^{-3}$ for different values of the s-wave scattering length

Looking at this dispersion relation, we see that if there be some interesting behaviour in the dispersion relation, the factors a and n will play a key role. We display two graphs of the dispersion relation, first, which keeps the particle density n fixed and varies the scattering length a and second, which keeps the scattering length fixed and changes the density. For the first case, keeping the density fixed at $n = 10^{15} \text{ cm}^{-3}$ we get the plot in Fig.(1) for certain values of the scattering length a . This figure shows that to observe the roton minimum, we have

the spectrum of elementary excitations on top of this uniform density state. For this purpose we do a linear stability analysis around the uniform density ground state using elementary excitations of the form $\theta(\mathbf{r}, t) = \sum_i [u_i(\mathbf{r}) e^{-\frac{i\omega_i t}{\hbar}} + v_i^*(\mathbf{r}) e^{\frac{i\omega_i t}{\hbar}}] e^{-i\mu t/\hbar}$ with $u_i(\mathbf{r}) = u_i e^{i\mathbf{k} \cdot \mathbf{r}}$ and $v_i(\mathbf{r}) = v_i e^{i\mathbf{k} \cdot \mathbf{r}}$. Working in cartesian coordinates, using $\psi(\mathbf{r}, t) = \psi_0(\mathbf{r}, t) + \theta(\mathbf{r}, t)$ and substituting this in Eq.(1) we get the following matrix, by separating terms with $e^{-\frac{i\omega_i t}{\hbar}}$ and those with $e^{\frac{i\omega_i t}{\hbar}}$

to increase the range of interactions given by the s-wave scattering length beyond the average inter-particle distance. This can be achieved by using the technique of Feshbach resonance to increase the s-wave scattering length[7]. Secondly, we fix the scattering length at $a = 10^{-5} \text{ cm}$ and plot the dispersion relation for certain values of density, shown in Fig.(2). This plot shows that for the roton minimum to be visible, we have to make the density large. So, we can say by looking at both these figures that for the roton minimum to be present, the range of interactions has to be larger than the average interparticle separation, as in liquid He II.

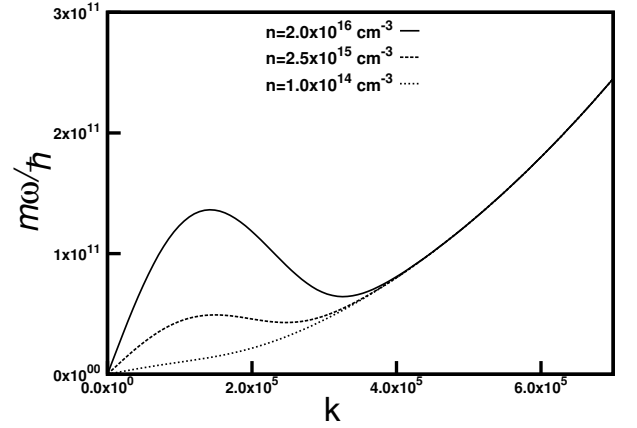


FIG. 2. Figure shows the dispersion relation at a fixed value of s-wave scattering length $a = 10^{-5} \text{ cm}$, for different values of density of the condensate.

Note that in the above discussion we could have just considered excitations along one axis and obtained exactly the same dispersion relation. In this regard, we use the series expansion of the order parameter presented in the previous section in Eq.(3) and go through the process of calculating the dispersion relation as has been

done above. The dispersion relation series thus obtained is

$$\omega^2 = \frac{\hbar^2}{m^2} \left[\frac{k^4}{4} + 4\pi a n k^2 \left(1 - \frac{a^2 k^2}{2} + \frac{a^4 k^4}{8} - \frac{a^6 k^6}{48} + \frac{a^8 k^8}{384} - \dots \right) \right]. \quad (9)$$

The dispersion relation obtained at various levels of truncation of the above Eq.(9) can be seen in Fig.(3). This figure shows the qualitative appearance of the roton minimum while just considering the first few terms. Note here that we have to terminate the series only when the coefficient of the leading order term in k in the expansion is positive, since otherwise ω would not be real beyond a certain value of k . Fig.(3) shows the power of the perturbative expansion in explaining at least the qualitative features of the elementary excitations here in particular. This perturbative expansion may be used to study other features of non-local interactions to unearth many qualitative features of systems where the exact analytical solution may not be available and also where the form of the non-local inter-atomic interaction potential may be different, but still satisfies the criteria $\int V_{eff}(\mathbf{r})d\mathbf{r} = g$.

The Gaussian interaction is a convenient representation of the flat and smooth V_{eff} . The interaction potential doesn't necessarily require a Gaussian profile. An adequate smoothness of the flat potential can be obtained even not going up to very high order in Taylor series and the present analysis shows that is enough for roton minimum.

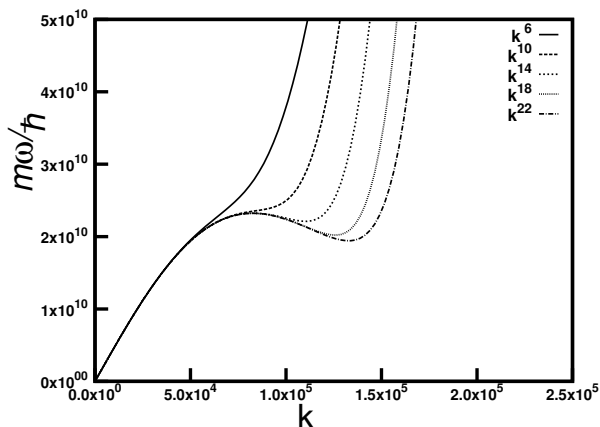


FIG. 3. Figure shows the dispersion relation at a fixed value of s-wave scattering length $a = 1.75 \times 10^{-5} \text{ cm}$, density $n = 10^{-15} \text{ cm}^{-3}$, for different orders of truncation of the perturbative GP equation for elementary excitations in Eq.(9). The labels in the figure indicate the leading order term in k kept in the Taylor expansion.

DISCUSSION

In the present paper, we have analysed two aspects of the effect of non-local interactions in a free Bose-Einstein condensate. These are, the energy functional of the truncated Taylor series expansion of non-local GP equation where the inter-atomic potential is non-contact type, and the small amplitude oscillations on top of the uniform density ground state in the presence of such a non-local inter-atomic potential. We have considered the long-range s-wave scattering of particles.

We have taken a perturbative scheme to find higher order corrections to the GP equation in the presence of non-local interactions, which was previously done by us[4]. As we see from the series expansion, the coefficients of the terms with higher order derivatives of $|\psi|^2$ fall off for $a < 1$ and hence it can be used for BEC systems whose density does not vary very rapidly. The exact correspondence between the terms in the expansion of the GP energy functional and the modified GP equation, in the presence of inter-atomic interaction potentials which give only even order derivatives in the expansion in general, presents a non-trivial feature of this expansion. Further the outcome of the combinatorial proof presented also states that if the interaction potential allows for the derivatives with odd order to be present, the higher order terms in the modified GP dynamics don't correspond to the higher order terms in the expansion of the GP energy functional. While there might exist functionals whose variation with respect to ψ^* gives terms which correspond to $\psi \partial_x^l (|\psi|^2)$ with odd l , it is peculiar to note that the variation of terms in the Taylor expansion of the GP energy functional of the form $\frac{\psi}{2} \partial_x^l (|\psi|^2)$ with odd l do not have any contribution to the modified GP equation. Further, we also propose that such a perturbative expansion with a definite energy functional may be used to study qualitative features of BEC systems with non-local, but integrable interatomic potentials.

From the analysis of the small amplitude oscillations on top of the uniform density ground state, it comes out that there appears a roton minimum by keeping the s-wave scattering length constant and varying the density and vice versa. By studying its gradual appearance it turns out that for the dispersion relation to show a roton minimum the s-wave scattering length, which gives the inter-atomic interaction range in our model, should be greater than the average inter-particle distance. Hence, the diluteness condition $a^3 n \ll 1$ needs to be relaxed for roton minimum to appear. Due to the violation of the diluteness criteria, 3 body effects would come into the picture, but since two body interactions would still exist, we may expect to see the roton minimum. In superfluid He II due to large density, the range of interatomic interactions is larger than the average inter-particle separation. Thus the case of superfluid He II may be thought of as

the regime of BEC beyond the diluteness criterion, but which still can be treated roughly by the GP equation.

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